Restoration of three-dimensional correlation function and structure factor from two-dimensional observations

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The static pair correlation (distribution) function and the structure factor of particle distributions in three-dimensional homogeneous isotropic systems are explicitly restored from two-dimensional data observed in a thin slab sliced out from original systems. While two-dimensional values for given thickness of the slab are readily calculated from three-dimensional functions, one would like to make the reverse in usual experiments by, for example, scanning the slab perpendicularly. Such a reconstruction is also possible even without scanning and three-dimensional pair correlation function and the structure factor are expressed by two-dimensional data in the form of an expansion with respect to the thickness of the slab. As an application, the behavior of the structure factor corresponding to the critical fluctuation is discussed. These results are expected to be useful when three-dimensional systems are observed by the illumination of thin planar lasers.

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I. INTRODUCTION

Statistical properties of particle systems are described by various correlation functions in the real space and corresponding spectra in the Fourier space. Experimental observations of these functions and spectra are usually performed under limited conditions and it is necessary to evaluate them based on restricted information. This paper is intended to contribute to one of such reconstructions, the evaluation of the three-dimensional static pair correlation (distribution) function and the structure factor from those obtained by two-dimensional observations.

We consider a three-dimensional system of particles and make a two-dimensional observation of a part of the system which is cut out as a slice. This situation is common for experiments where particles are observed by the scattering of the thin planar laser beam or by the fluorescence induced by them. For example, in fine particle (dusty) plasma experiments, the main target of observation is the behavior of fine particles (dusts) and their orbits are recorded by CCD cameras through scattering of illuminating planar laser beams[1]. If the system is stationary and the timescale of the target phenomena is long enough, one can obtain three-dimensional data by scanning the beam perpendicularly to the sheet of the beam. We may have, however, many cases where the latter is not available.

Our basic assumption is the statistical homogeneity and isotropy of the system. We also assume the threshold of detection by the light beam is adjusted so that all particles located within a given thickness are recorded and we have their two-dimensional positional data in the plane of the beam. It is trivial that values of the two-dimensional pair correlation function and the structure factor obtained by two-dimensional observations are determined by three-dimensional values. We emphasize that, under the assumption of the homogeneity and isotropy, the reverse is also true: *the three-dimensional pair correlation (distribution) function and the structure factor can be reproduced from two-dimensional results.* We have shown the inverse formula for the pair correlation (distribution) function in the form of an expansion with respect to the thickness of the beam[2]. We here derive the relations for the structure factors (which have more mathematical aspects than those for correlation functions) and give a simple application of the result.

II. CORRELATION FUNCTIONS AND STRUCTURE FACTORS IN THREE AND TWO DIMENSIONS

We take the origin of coordinates at the center of the thickness of detection with the xy-plane and the z-axis parallel and perpendicular to the beam sheet, respectively. The system has N particles in the volume $V = SL_z$ where $S = L_xL_y$ is the area of the base parallel to the xy-plane and L_z is the height in the z-direction. The thickness and

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the volume of the sliced part detected by the beam are b and Sb, respectively. We denote the number of particles in the observed domain by N_{2d} which is related to N by

$$N_{2d} = (b/L_z)N. \tag{2.1}$$

We denote three- and two-dimensional coordinates by $\mathbf{r} = (x, y, z) = (\mathbf{R}, z)$ and $\mathbf{R} = (x, y)$, respectively. We also denote three- and two-dimensional wave numbers by $\mathbf{k} = (k_x, k_y, k_z) = (\mathbf{K}, k_z)$ and $\mathbf{K} = (k_x, k_y)$, respectively.

The microscopic number densities in three and two dimensions, $\rho(\mathbf{r};\ 3d)$ and $\rho(\mathbf{R};\ 2d)$, are defined by

$$\rho(\mathbf{r};\ 3d) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) = \sum_{i=1}^{N} \delta(\mathbf{R} - \mathbf{R}_i)\delta(z - z_i) \tag{2.2}$$

and

$$\rho(\mathbf{R};\ 2d) = \int_{-b/2}^{b/2} dz \rho(\mathbf{r};\ 3d), \tag{2.3}$$

respectively. The pair correlation functions in three and two dimensions, $h(r;\ 3d)$ and $h(R;\ 2d)$, are defined respectively by

$$< \rho(\mathbf{r};\ 3d)\rho(\mathbf{r}';\ 3d) >= \frac{N}{V}\delta(\mathbf{r} - \mathbf{r}') + \left(\frac{N}{V}\right)^2 [1 + h(|\mathbf{r} - \mathbf{r}'|;\ 3d)] \tag{2.4}$$

and

$$< \rho(\mathbf{R};\ 2d)\rho(\mathbf{R}';\ 2d) >= \frac{N_{2d}}{S}\delta(\mathbf{R} - \mathbf{R}') + \left(\frac{N_{2d}}{S}\right)^2 [1 + h(|\mathbf{R} - \mathbf{R}'|;\ 2d)], \tag{2.5}$$

where $<\ >$ denotes the statistical average. These pair correlation functions are related to each other in the same way as the pair distribution functions[2]. The two-dimensional correlation function is expressed by the three-dimensional one as

$$h(R;\ 2d) \approx h\left[R\left(1 + \frac{1}{12}\frac{b^2}{R^2} - \frac{1}{120}\frac{b^4}{R^4}\right);\ 3d\right] + \frac{7}{1440}\frac{b^4}{R^4}R^2\frac{d^2h(R;\ 3d)}{dR^2}, \qquad \frac{b}{R} < 1. \tag{2.6}$$

Inversely, the three-dimensional correlation function is expressed by the two-dimensional one as

$$h(r;\ 3d) \approx h\left[r\left(1 - \frac{1}{12}\frac{b^2}{r^2} + \frac{1}{720}\frac{b^4}{r^4}\right);\ 2d\right] - \frac{7}{1440}\frac{b^4}{r^4}r^2\frac{d^2h(r;\ 2d)}{dr^2}, \qquad \frac{b}{r} < 1. \tag{2.7}$$

We derive similar relations for the structure factors.

In three dimensions, the Fourier component of the number density $\tilde{\rho}(\mathbf{k};\ 3d)$ is defined by

$$\tilde{\rho}(\mathbf{k};\ 3d) = \int_V d\mathbf{r} \exp(-i\mathbf{k}\cdot\mathbf{r})\rho(\mathbf{r};\ 3d) \tag{2.8}$$

and the inverse Fourier transform is given by

$$\rho(\mathbf{r};\ 3d) = \frac{1}{V}\sum_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{r})\tilde{\rho}(\mathbf{k};\ 3d), \tag{2.9}$$

where

$$\mathbf{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right), \quad n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots. \tag{2.10}$$

In two dimensions, the Fourier component of the number density $\tilde{\rho}(\mathbf{K};\ 2d)$ is defined by

$$\tilde{\rho}(\mathbf{K};\ 2d) = \int_S d\mathbf{R} \exp(-i\mathbf{K}\cdot\mathbf{R})\rho(\mathbf{R};\ 2d) \tag{2.11}$$

and the inverse Fourier transform is given by

$$\rho(\mathbf{R};\ 2d) = \frac{1}{S}\sum_{\mathbf{K}} \exp(i\mathbf{K}\cdot\mathbf{R})\tilde{\rho}(\mathbf{K};\ 2d), \tag{2.12}$$

where

$$\mathbf{K} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}\right), \quad n_x, n_y = 0, \pm 1, \pm 2, \ldots. \tag{2.13}$$

In three and two dimensions, the structure factors are defined respectively by

$$S(\mathbf{k};\ 3d) = S(k;\ 3d) = \frac{1}{N} < |\tilde{\rho}(\mathbf{k};\ 3d)|^2 > \tag{2.14}$$

and

$$S(\mathbf{K};\ 2d) = S(K;\ 2d) = \frac{1}{N_{2d}} < |\tilde{\rho}(\mathbf{K};\ 2d)|^2 > . \tag{2.15}$$

The correlation functions are related to structure factors by

$$h(r;\ 3d) = \frac{1}{(2\pi)^3(N/V)}\int d\mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{r})[S(k;\ 3d) - 1] \tag{2.16}$$

and

$$h(R;\ 2d) = \frac{1}{(2\pi)^2(N_{2d}/S)}\int d\mathbf{K}\exp(i\mathbf{K}\cdot\mathbf{R})[S(K;\ 2d) - 1]. \tag{2.17}$$

Here, the sums over wave numbers are rewritten into the integrals assuming V and S are sufficiently large. Similar limits will be taken in what follows when possible without ambiguity.

III. CONVERSION OF THREE-DIMENSIONAL STRUCTURE FACTOR INTO TWO DIMENSIONS

The density fluctuation in two dimensions $\tilde{\rho}(\mathbf{K};\ 2d)$ is related to the three-dimensional one by

$$\tilde{\rho}(\mathbf{K};\ 2d) = \int_S d\mathbf{R}\exp(-i\mathbf{K}\cdot\mathbf{R})\int_{-b/2}^{b/2} dz\rho(\mathbf{r};\ 3d) = \frac{b}{L_z}\sum_{k_z}\tilde{\rho}(\mathbf{K}, k_z;\ 3d)\left(\frac{\sin(k_z b/2)}{k_z b/2}\right) \tag{3.1}$$

and $S(K;\ 2d)$ is calculated from $S(k;\ 3d)$ as

$$\begin{aligned} S(K;\ 2d) &= \frac{1}{N_{2d}} < |\tilde{\rho}(\mathbf{K};\ 2d)|^2 > \\ &= \frac{b}{2\pi}\int_{-\infty}^{\infty} dk_z S(k = (K^2 + k_z^2)^{1/2};\ 3d)\left(\frac{\sin(k_z b/2)}{k_z b/2}\right)^2 . \end{aligned} \tag{3.2}$$

We thus have

$$\begin{aligned} S(K;\ 2d) &= \frac{b}{2\pi}\int_{-\infty}^{\infty} dk_z S(k;\ 3d)\left(\frac{\sin(k_z b/2)}{k_z b/2}\right)^2 \\ &= \frac{b}{\pi}\int_K^{\infty} dk\frac{k}{(k^2 - K^2)^{1/2}} S(k;\ 3d)\left(\frac{\sin[(k^2 - K^2)^{1/2}b/2]}{(k^2 - K^2)^{1/2}b/2}\right)^2 . \end{aligned} \tag{3.3}$$

Since

$$\frac{b}{2\pi}\int_{-\infty}^{\infty} dk_z\left(\frac{\sin(k_z b/2)}{k_z b/2}\right)^2 = 1,$$

this relation is rewritten into the form

$$\begin{aligned} S(K;\ 2d)-1 &= \frac{b}{2\pi}\int_{-\infty}^{\infty} dk_z[S(k;\ 3d)-1]\left(\frac{\sin(k_z b/2)}{k_z b/2}\right)^2 \\ &= \frac{b}{\pi}\int_{K}^{\infty} \frac{dkk}{(k^2-K^2)^{1/2}}[S(k;\ 3d)-1]\left(\frac{\sin[(k^2-K^2)^{1/2}b/2]}{(k^2-K^2)^{1/2}b/2}\right)^2 . \end{aligned} \tag{3.4}$$

When expanded with respect to b, we have

$$S(K;\ 2d)-1 = \frac{b}{\pi}\int_{K}^{\infty} \frac{dkk}{(k^2-K^2)^{1/2}}\left[1-\frac{b^2}{12}(k^2-K^2)+\frac{b^4}{360}(k^2-K^2)^2\right][S(k;\ 3d)-1] \tag{3.5}$$

to the order b^4.

The relation (3.3) or (3.4) should be derived also from the relation between correlation functions in the real space (2.6). When we neglect terms proportional to b^2 or b^4 in (2.6) assuming b is sufficiently small, we have

$$h(R;\ 2d) \approx h(R;\ 3d). \tag{3.6}$$

We then have

$$\begin{aligned} S(K;\ 2d)-1 &= 2\pi\frac{N_{2d}}{S}\int dRRJ_0(KR)h(R;\ 2d) \\ &\approx 2\pi\frac{N_{2d}}{S}\int dRRJ_0(KR)h(R;\ 3d) \\ &= \frac{b}{\pi}\int_0^{\infty} dRRJ_0(KR)\int_0^{\infty} dkk^2\frac{\sin(kR)}{kR}[S(k;\ 3d)-1]. \end{aligned} \tag{3.7}$$

Noting that

$$\int_0^{\infty} dRR\frac{\sin(kR)}{kR}J_0(KR) = \frac{1}{k(k^2-K^2)^{1/2}}\theta(k-K), \tag{3.8}$$

we have

$$S(K;2d)-1 = \frac{b}{\pi}\int_K^{\infty}\frac{dkk}{(k^2-K^2)^{1/2}}[S(k;\ 3d)-1], \tag{3.9}$$

which is the $b \to 0$ limit of (3.4) (Since $S(k;\ 3d) \to 1$ as $k \to \infty$, we have to treat this limiting value of $S(k;\ 3d)$ separately for the convergence of the integral).

IV. INVERSE RELATIONS FOR STRUCTURE FACTORS

In the real space, we have the inverse relation (2.7) for the correlation function. In the small b limit, we have

$$h(r;\ 3d) \approx h(r;\ 2d). \tag{4.1}$$

This gives

$$\begin{aligned} S(k;\ 3d)-1 &= \frac{N}{V}4\pi\int_0^{\infty} drr^2\frac{\sin(kr)}{kr}h(r;\ 3d) \\ &\approx \frac{N}{V}4\pi\int_0^{\infty} drr^2\frac{\sin(kr)}{kr}h(r;\ 2d) \\ &= \frac{2}{b}\int_0^{\infty} drr^2\frac{\sin(kr)}{kr}\int_0^{\infty} dKKJ_0(Kr)[S(K;\ 2d)-1] \\ &= -\frac{2}{b}\int_0^{\infty} drr\frac{\sin(kr)}{kr}\int_0^{\infty} dKKJ_1(Kr)\frac{d}{dK}[S(K;\ 2d)-1]. \end{aligned} \tag{4.2}$$

Noting that

$$\int_0^\infty drr\frac{\sin(kr)}{kr}J_1(Kr) = \frac{1}{K(K^2-k^2)^{1/2}}\theta(K-k), \tag{4.3}$$

we have

$$S(k;\ 3d) - 1 = -\frac{2}{b}\int_k^\infty dK\frac{1}{(K^2-k^2)^{1/2}}\frac{d}{dK}[S(K;\ 2d)-1]. \tag{4.4}$$

Equation (4.4) is the inverse of the relation (3.9) as is also directly checked by substituting (4.4) into (3.9):

$$\begin{aligned}
&\frac{b}{\pi}\int_K^\infty \frac{dkk}{(k^2-K^2)^{1/2}}\left[-\frac{2}{b}\int_k^\infty dK'\frac{1}{(K'^2-k^2)^{1/2}}\frac{d}{dK'}[S(K';\ 2d)-1]\right] \\
&= -\frac{2}{\pi}\int_K^\infty dK'\frac{d}{dK'}[S(K';\ 2d)-1]\int_K^{K'}\frac{dkk}{(k^2-K^2)^{1/2}}\frac{1}{(K'^2-k^2)^{1/2}} \\
&= -\int_K^\infty dK'\frac{d}{dK'}[S(K';\ 2d)-1] = S(K;\ 2d)-1.
\end{aligned} \tag{4.5}$$

Equations (3.9) and (4.4) give the transformations from $S(k;\ 3d)$ to $S(K;\ 2d)$ and vise versa in the lowest order in b. While (3.3) or (3.4) gives exact values of $S(K;\ 2d)$ including higher order terms, the purpose of experiments is to obtain values of $S(k;\ 3d)$ from those of $S(K;\ 2d)$. Let us now derive higher order terms in the inverse formula for $S(k;\ 3d)$.

Since the inverse of (3.4) is given by (4.4) in the lowest order, we put

$$S(k;\ 3d) - 1 = \frac{1}{b}\left[-2\int_k^\infty \frac{dK}{(K^2-k^2)^{1/2}}\frac{d}{dK}[S(K;\ 2d)-1] + b^2\Delta^{(2)}(k) + b^4\Delta^{(4)}(k)\right] \tag{4.6}$$

and determine $\Delta^{(2)}(k)$ and $\Delta^{(4)}(k)$ so as to satisfy (3.5). Substituting (4.6) into (3.5) and noting (4.5), we have

$$\begin{aligned}
&\int_K^\infty \frac{dkk}{(k^2-K^2)^{1/2}}\Delta^{(2)}(k) \\
&= -\frac{1}{6}\int_K^\infty dkk(k^2-K^2)^{1/2}\int_k^\infty \frac{dK'}{(K'^2-k^2)^{1/2}}\frac{d}{dK'}[S(K';\ 2d)-1]
\end{aligned} \tag{4.7}$$

and

$$\begin{aligned}
&\int_K^\infty \frac{dkk}{(k^2-K^2)^{1/2}}\Delta^{(4)}(k) = \frac{1}{12}\int_K^\infty dkk(k^2-K^2)^{1/2}\Delta^{(2)}(k) \\
&+ \frac{1}{180}\int_K^\infty dkk(k^2-K^2)^{3/2}\int_k^\infty \frac{dK'}{(K'^2-k^2)^{1/2}}\frac{d}{dK'}[S(K';\ 2d)-1]
\end{aligned} \tag{4.8}$$

in the orders b^2 and b^4, respectively.

Rewriting the right-hand side of (4.7) as

$$\begin{aligned}
&-\frac{1}{6}\int_K^\infty dK'\frac{d}{dK'}[S(K';\ 2d)-1]\int_K^{K'} dkk\frac{(k^2-K^2)^{1/2}}{(K'^2-k^2)^{1/2}} \\
&= -\frac{\pi}{24}\int_K^\infty dK'(K'^2-K^2)\frac{d}{dK'}[S(K';\ 2d)-1] = \frac{\pi}{12}\int_K^\infty dK'K'[S(K';\ 2d)-1]
\end{aligned} \tag{4.9}$$

and noting that the inverse of (3.9) is given by (4.4), we can solve (4.7) for $\Delta^{(2)}(k)$ in the form

$$\begin{aligned}
\Delta^{(2)}(k) &= -\frac{2}{b}\int_k^\infty \frac{dK}{(K^2-k^2)^{1/2}}\frac{d}{dK}\left[\frac{b}{12}\int_K^\infty dK'K'[S(K';\ 2d)-1]\right] \\
&= \frac{1}{6}\int_k^\infty \frac{dK}{(K^2-k^2)^{1/2}}K[S(K;\ 2d)-1].
\end{aligned} \tag{4.10}$$

Substituting (4.10) into (4.8), we have

$$\int_K^\infty \frac{dkk}{(k^2-K^2)^{1/2}}\Delta^{(4)}(k)$$

$$=\frac{1}{72}\int_K^\infty dkk(k^2-K^2)^{1/2}\int_k^\infty \frac{dK'}{(K'^2-k^2)^{1/2}}K'[S(K';\ 2d)-1]$$

$$+\frac{1}{180}\int_K^\infty dkk(k^2-K^2)^{3/2}\int_k^\infty \frac{dK'}{(K'^2-k^2)^{1/2}}\frac{d}{dK'}[S(K';\ 2d)-1].$$

The right-hand side is rewritten as

$$\frac{1}{72}\int_K^\infty dK'K'[S(K';\ 2d)-1]\int_K^{K'} dkk\frac{(k^2-K^2)^{1/2}}{(K'^2-k^2)^{1/2}}$$

$$+\frac{1}{180}\int_K^\infty dK'\frac{d}{dK'}[S(K';\ 2d)-1]\int_K^{K'} dkk\frac{(k^2-K^2)^{3/2}}{(K'^2-k^2)^{1/2}}$$

$$=-\frac{\pi}{1440}\int_K^\infty dK'(K'^2-K^2)K'[S(K';\ 2d)-1]$$

and (4.8) is solved for $\Delta^{(4)}(k)$ in the form

$$\begin{aligned}\Delta^{(4)}(k) &= \frac{1}{720}\int_k^\infty \frac{dK}{(K^2-k^2)^{1/2}}\frac{d}{dK}\int_K^\infty dK'(K'^2-K^2)K'[S(K';\ 2d)-1]\\ &= -\frac{1}{360}\int_K^\infty dK'K'[S(K';\ 2d)-1]\int_k^{K'}\frac{dKK}{(K^2-k^2)^{1/2}}\\ &= -\frac{1}{360}\int_k^\infty dKK(K^2-k^2)^{1/2}[S(K;\ 2d)-1].\end{aligned} \tag{4.11}$$

Substituting (4.10) and (4.11) into (4.6), we have finally

$$S(k;\ 3d)-1=\int_k^\infty \frac{dK}{(K^2-k^2)^{1/2}}\left[-\frac{2}{b}\frac{d}{dK}+\frac{b}{6}K-\frac{b^3}{360}K(K^2-k^2)\right][S(K;\ 2d)-1] \tag{4.12}$$

as the inverse of (3.5).

V. APPLICATION

One of remarkable phenomena observed in the static structure factors may be the density fluctuations near the critical point: When the critical point is approached, an enhancement and eventual divergence are expected in the spectrum of long wavelength density fluctuations[3]. A possibility of the critical point has been pointed out in fine particle plasmas[4, 5] where particle orbits are usually observed by thin laser beams and the behavior of density fluctuations near the critical point has been calculated[5]. We here show how such a divergence looks in two-dimensional images.

Let us assume that the three-dimensional structure factor shows the critical behavior at long wavelengths in the form

$$S(k;\ 3d)\sim\frac{1}{c^2+(k/k_0)^2},\qquad k\to 0 \tag{5.1}$$

with $c^2\to 0$ at the critical point. When observed by the laser beam of thickness b, the two-dimensional structure factor takes the form given by (3.3). If b is sufficiently small, we have

$$S(K;\ 2d)\sim\frac{bk_0}{2}\frac{1}{(c^2+K^2/k_0^2)^{1/2}}. \tag{5.2}$$

The two-dimensional structure factor observed by the laser beam of thickness b has a *weaker divergence* in proportion to c as

$$S(K;\ 2d) \sim \frac{bk_0}{2c}, \qquad K \to 0 \tag{5.3}$$

in comparison with the (true) three-dimensional one

$$S(k;\ 3d) \sim \frac{1}{c^2}, \qquad k \to 0, \tag{5.4}$$

while the wave number characterizing the behavior in K-space is k_0, the same as the three-dimensional behavior.

At long wavelengths, two-dimensional results takes the form

$$\frac{1}{S(K;\ 2d)^2} \sim C_1^2 + K^2/K_0^2 \tag{5.5}$$

with

$$C_1^2 = \left(\frac{2}{bk_0}\right)^2 c^2 \tag{5.6}$$

and

$$K_0 = \frac{bk_0^2}{2}. \tag{5.7}$$

We thus have

$$c^2 = \frac{bK_0}{2} C_1^2 \tag{5.8}$$

and

$$k_0^2 = 2\frac{K_0}{b}. \tag{5.9}$$

These equations give c^2 and k_0 of the true structure factor $S(k;\ 3d)$ in terms of the values obtained by two-dimensional observations, C_1^2 and K_0, and the (known) value of the beam thickness b.

VI. CONCLUSION

In addition to those for the correlation (distribution) functions, the relations between the three- and two-dimensional structure factors are given. It is obvious that, when the three-dimensional structure factor is known for homogeneous and isotropic systems, we can calculate the values of two-dimensional structure factor observed in a slab sliced out from three-dimensional systems. It is shown that the reverse is also possible: The three-dimensional structure factor is expressed by the values of two-dimensional one in the form of an expansion with respect to the thickness of the slab. The results is applied to the case of critical density fluctuations expected in the structure factor near the critical point. Characteristic parameters of critical fluctuations are related to those observed in two-dimensional structure factor, enabling estimation of the former by two-dimensional observations.

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